

# A Scaling Algorithm of Self-avoiding Chain Adsorbed on the Surface

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**Abstract**— A single polymer chain with one end tethered to an impenetrable flat surface is simulated by using Monte Carlo simulation method. The polymer chain is generated using self-avoiding walk method in the simple cubic lattice. The monomer does Brownian motion by the bond-fluctuation method in the simulation. After a long Monte Carlo step, the conformation of the chain reaches equilibrium. There is a scaling relation between the surface contact number  $M$  and the chain length  $N$  at the critical adsorption temperature  $T_c$ . The scaling algorithm is presented to determine the critical adsorption point  $T_c$  by the variance between the interpolation value and the curve fitting value. The dependence of the surface contact number  $M$  on the chain length  $N$  is presented near the critical adsorption point  $T_c$  by two critical exponents  $\phi$  and  $\delta$ . The results provide a new efficient method to locate the critical adsorption point and to find out the critical exponents.

**Index Terms**—simulation, chain, critical adsorption, scaling method

## I. INTRODUCTION

The critical adsorption of polymer chain on the surface is a hot research topic for polymer science, bioinformatics and other aspects [1-3]. The adsorption of polymers is complex and is influenced by many factors. The adsorption mechanism is still not well explained by the research achievements. The studies are often carried out by means of computer modeling. The simplest model is a linear polymer chain which is made up of a large number of monomers with the same structure as concatenation. The monomers move or rotate for their thermal motion which changes the conformation constantly. The

molecular weight of the polymer chain is always large, so the number of conformations is also very large for long polymer chain. Hence, the conformation statistics of a single polymer chain is a complex computational problem and is often performed by computer simulation. The conformation and the shape of the chain depend on the solvent, and the environmental factors such as the temperature, which increases the complexity of the chain conformation.

The behavior of the polymer chains on the interface can be applied to many fields, such as water treatment, solid-liquid separation and pharmaceutical materials. The study of polymer adsorption has important scientific and application value for life sciences, pharmaceutical sciences, materials science and other fields. The behavior of the polymer chains in the interface is an important research direction of material science, information science, biology and other fields [4-12].

The conformation of polymer is not only related to the structure of the molecule itself, but also related to external conditions, such as solvent, temperature, and the surface material. In this paper, self-avoiding walk method is used to simulate the polymer chain. And then we use the bond fluctuation model to simulate the random thermal motion of monomers. The monomer in contact with the surface has an attraction interaction, which is related to the temperature. Monte Carlo method is used to simulate the conformational properties of self-avoiding chain in different temperatures. We analyze the computer simulation data and calculate the critical adsorption temperature by the improved EKB (Eisenriegler, Kremer, and Binder) scale algorithm [6]. We interpolate some values between the simulation sample data and then do linear fit to calculate the critical adsorption temperature and the crossover exponents. We found that two exponents can be better to represent the surface contact number near the critical adsorption point than that of one exponent.

Manuscript received May 15, 2013; revised Nov. 25, 2013; accepted Dec. 1, 2013.

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## II. ALGORITHM OF SIMULATION CHAIN

### A. Three-dimensional Lattice Space Model

Three-dimensional space  $L_x \times L_y \times L_z$  is presented as the cubic grid space  $G(x, y, z)$  by the simple cubic lattice. In this cubic lattice model, each lattice point can be occupied by one monomer. The space coordinates  $(x, y, z)$  of monomers are confined at the lattice point. The periodic boundary conditions are performed in the  $x, y$  directions. An infinite large surface is placed at  $z = 0$ , and is not to be crossed by chain. All monomers in the chain are located above the surface ( $z > 0$ ).

### B. Chain Growth Model

Polymer chain is made up of many monomers that are joined together one by one. The chain length  $N$  means the polymer chain with  $N$  repeating monomers. If all the repeating monomers belong to one type, the polymer chain is referred as a homogenous polymer. In this paper, we consider only homogenous polymer chain. Linear polymer chain is the simplest structure without any branches. The monomers are joined together with the bond length and the rotation angle. From the perspective of the computer simulation, the polymer chain, which contains  $N$  repeating units, is generated by walking  $N$  step as shown in Fig. 1.

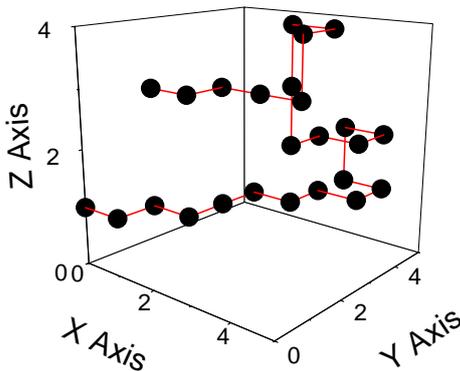


Figure 1 The sketch of a self-avoiding chain in 3D space.

Each lattice point can only be occupied by one monomer in the lattice chain model, so the monomer walking method is known as self-avoiding walk (SAW). At some time, the conformation of polymer chain is completely random. So Monte Carlo method is performed as follows:

Step 1: Initialize all the grid space  $G(x, y, z) = 0$  ( $x, y, z$  for the coordinate of space lattice). The first monomer of the chain is fixed at the grid points  $(0,0,1)$ , i.e.  $G(0,0,1) = 1$ , then the chain grows step by step using self-avoiding walk in the cubic lattice space with the walking step unit.

Step 2: The  $n$ -th monomer walking direction  $k_n$  is generated randomly according to

$$k_n = \text{INT}[(b-a+1) * r_n] + a \quad (1)$$

from the integer sequence among  $[a, b]$ . Each lattice has six nearest neighbors in three-dimensional cubic space, so we set  $a = 1$  and  $b = 6$ . Then an integer  $k_n$  generates randomly among  $[1, 6]$  as a walk direction and the

pseudo-random number  $r_n$  belong to  $(0, 1)$ . INT is a rounding function.

Step 3: The position of  $(n + 1)$ -th monomer is decided by the  $n$ -th monomer position and the direction to walk. The coordinate position of  $(n + 1)$ -th monomer is presented as  $(x_{n+1}, y_{n+1}, z_{n+1}) = (x_n + \Delta x, y_n + \Delta y, z_n + \Delta z)$ , where  $(x_n, y_n, z_n)$  is the  $n$ -th monomer coordinate,  $(\Delta x, \Delta y, \Delta z)$  is the shift of the  $n$ -th monomer. The walking direction  $k_n$  is corresponding to the shift as shown in Table I.

TABLE I.  
THE WALKING DIRECTION AND THE SHIFT VALUE.

$k_n$	$(\Delta x, \Delta y, \Delta z)$
1	(1, 0, 0)
2	(-1, 0, 0)
3	(0, 1, 0)
4	(0, -1, 0)
5	(0, 0, 1)
6	(0, 0, -1)

Step 4: Overlap is ascertained by whether the lattice is occupied by more than one monomer, which can be described as the follows:

```

if ( $G(x_{n+1}, y_{n+1}, z_{n+1}) == 0$ )
    { /* walking success*/
         $G(x_{n+1}, y_{n+1}, z_{n+1}) = n+1$ ;
         $n = n + 1$ ;
         $n_{try} = 0$ ;
    }
else
    { /* walking failure*/
         $n_{try} = n_{try} + 1$ ;
        if ( $n_{try} > 2 * b$ )
            {  $G(x_n, y_n, z_n) = 0$ ;
               $n_{try} = 0$ ;
              if ( $n > 0$ )  $n = n - 1$ ;
            }
        }
    Exit the loop to re-walk, skip to step 2.
    }
    
```

Step 5: Repeat the above steps from step 2 to step 4 until all  $N$  monomers of the polymer chain generated. The conformation of linear chain is generated by self-avoiding walk in the three-dimensional space, as shown in Fig. 1.

### C. Bond Fluctuation and Chain Movement

Considering the fluctuation of the bond length, any nearest neighbor monomers are located at two vertices of one cubic lattice unit. The bond length between two nearest neighbor monomers may be one of three cases: the length of one side (1), the diagonal of one unit square ( $\sqrt{2}$ ) and the cube diagonal ( $\sqrt{3}$ ). The coordination number of each lattice is  $z = 26$ .

Every monomer does Brownian motion. The monomer may be to move one step at one of six coordinate axes directions which is selected randomly one of the

directions. Each monomer in contact with the surface, where the distance of the monomer from the surface is one unit, has an energy  $E$ . The trial move is accepted if all the following conditions are satisfied:

(a) The  $r$ -th monomer is selected randomly,  $r \in [2, N]$ .

(b) Six nearest neighbor lattices of the  $r$ -th monomer are detected whether they are free. And all the free lattices are recorded.

(c) The direction  $k$  is randomly selected from the free nearest neighbor lattices of the  $r$ -th monomer. The self-avoiding walking condition is satisfied after the trial move whether each lattice is occupied by up to only one monomer, which can be described as

if  $(G(x_r + \Delta x_k, y_r + \Delta y_k, z_r + \Delta z_k) \neq 0)$   
 {Skip to (a) and re-select the trial monomer. }

(d) Whether the new position of the  $r$ -th monomer is located above the surface is satisfied, which can be described as the follows:

if  $((z_r + \Delta z_k) \leq 0)$   
 {Skip to (a) and re-select the trial monomer. }

(e) Whether the bond between the  $r$ -th monomer and its nearest neighbors meets the allowable conditions of the bond length (1, sqrt (2), sqrt (3)) where  $|\dots|$  indicates the distance between two points, which can be described as the follows:

if  $(r > 1$  and  $(|G(x_r + \Delta x_k, y_r + \Delta y_k, z_r + \Delta z_k) - G(x_{r-1}, y_{r-1}, z_{r-1})| < 1$  or  $|G(x_r + \Delta x_k, y_r + \Delta y_k, z_r + \Delta z_k) - G(x_{r-1}, y_{r-1}, z_{r-1})| > \text{sqrt}(3))$ )  
 {Skip to (a) and re-select the trial monomer. }

if  $(r < N$  and  $(|G(x_r + \Delta x_k, y_r + \Delta y_k, z_r + \Delta z_k) - G(x_{r+1}, y_{r+1}, z_{r+1})| < 1$  or  $|G(x_r + \Delta x_k, y_r + \Delta y_k, z_r + \Delta z_k) - G(x_{r+1}, y_{r+1}, z_{r+1})| > \text{sqrt}(3))$ )  
 {Skip to (a) and re-select the trial monomer. }

(f)  $\Delta E$  is the energy shift before and after the move. The following conditions are satisfied.

If  $((\Delta E > 0)$  and  $(\exp(-\Delta E/k_B T) > r_n))$   
 {Skip to (a) and re-select the trial monomer. }

$r_n$  is a random number among (0, 1).  $k_B$  is the Boltzmann constant.

(g) At each trial movement, the counter may be auto-incremented once, which can be described as

counter = counter+1;  
 $G(x_r + \Delta x_k, y_r + \Delta y_k, z_r + \Delta z_k) = r$ ;  
 $G(x_r, y_r, z_r) = 0$ .

A Monte Carlo time step (MCS) means each monomer of the chain which attempts to move once.

If (counter == N)  
 $\{t = t + 1, \text{count} = 0\}$ .

The Monte Carlo Step is unit of movement time. Repeat (a) to (g) until the movement time  $t$  reaches the required time.

#### D. Model Parameters

In this paper, physical properties of self-avoiding chain are studied at the different temperature  $T$ . The program is performed from high temperature  $T = 6$  to low temperature  $T = 0.1$ . The temperature is reduced with step  $\Delta T$ . In this article,  $\Delta T$  is taken near at the critical adsorption point  $\Delta T = 0.05$ , but  $\Delta T$  slightly larger at other temperature. The conformation changes with MCS time.

Each sample runs the first time  $\tau = 2.5N^{2.13}$ MCS for relaxation and then runs  $100\tau$  MCS for statistic in which the physical properties are recorded at every  $0.1\tau$ .

### III. SCALING ALGORITHM OF CRITICAL ADSORPTION

#### A. Preliminary Estimates of the Critical Point $T_c$

In the previous study, the critical adsorption point (CAP) can be roughly estimated by the mean square end-to-end distance  $\langle R^2 \rangle$  and the mean square radius of gyration  $\langle R_g^2 \rangle$  that reaches a minimum near at the CAP [4-5]. We found  $T_c = 1.65 \pm 0.10$  where there is a minimal value of  $\langle R_g^2 \rangle$ , as shown in Fig. 2. The calculation method of the mean square gyration radius  $\langle R_g^2 \rangle$  can be expressed as

$$R_g^2 = \frac{1}{N} \sum_{i=1}^N [(x_i - x_c)^2 + (y_i - y_c)^2 + (z_i - z_c)^2], \quad (2)$$

where  $(x_i, y_i, z_i)$  is the coordinate of the  $i$ -th monomer and  $(x_c, y_c, z_c)$  is that of the center of polymer chain.

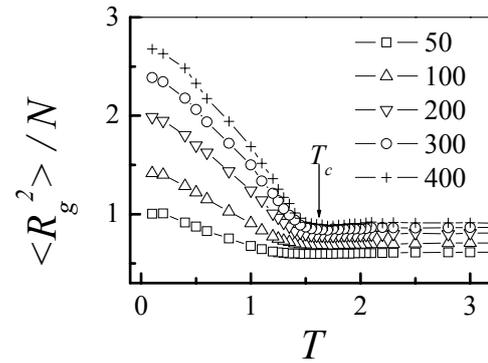


Figure 2 The dependence of the mean square radius of gyration  $\langle R_g^2 \rangle$  on the temperature  $T$ .

#### B. Scaling Method

The relation between the adsorption energy  $E$  and the number of monomers contacting with the surface  $M$  exists scaling relation  $E \sim M$ . The scaling relation is proposed between the energy  $E$  and the chain length  $N$  by Eisenriegler (EKB) [6], which can be expressed as

$$E(T) \propto \begin{cases} N^0 & (T \gg T_c) \\ N^\phi & (T = T_c) \\ N & (T \ll T_c) \end{cases} \quad (3)$$

At the critical adsorption point  $T_c$ , there is a relationship  $M \propto N^\phi$  between the surface contact number  $M$  and the chain length  $N$ . So the scaling relation between  $M$  and  $N$  is almost applicable at near  $T_c$ . To further determine the relationship among  $M$ ,  $N$  near  $T_c$ , we improve the algorithm based on EKB. We take five temperatures in the vicinity of the critical adsorption point  $T_c$ :  $T = 1.55, 1.60, 1.65, 1.70, \text{ and } 1.75$ . At  $T = T_c$ , the dependence of the surface contact number  $M$  on the chain length  $N$  can be expressed as

TABLE II.  
THE SIMULATION VALUE OF  $M(T, N)$

	10	50	100	150	200	250	300	400
1.75	3.63	7.56	9.99	11.72	12.95	13.98	14.77	16.07
1.70	3.69	7.99	10.91	13.21	14.53	15.79	17.11	18.97
1.65	3.76	8.48	11.88	14.44	16.52	18.4	20.22	22.97
1.60	3.83	9.06	13.15	16.34	19.19	21.79	23.98	28.6
1.55	3.92	9.7	14.71	18.84	22.53	25.98	29.13	35.48

$$M = a_0 N^\phi. \quad (4)$$

The surface contact number  $M(T, N)$  is enumerated for different chain length  $N$  at the different temperature near  $T_c$  in Table II. The first row represents the chain length  $N$ , which means that the temperature  $T$  lies in the first column. The other data in the table means the surface contacts number  $M(T, N)$ . The dual logarithmic relationship diagram between  $M$  and  $N$  is shown in Fig. 3.

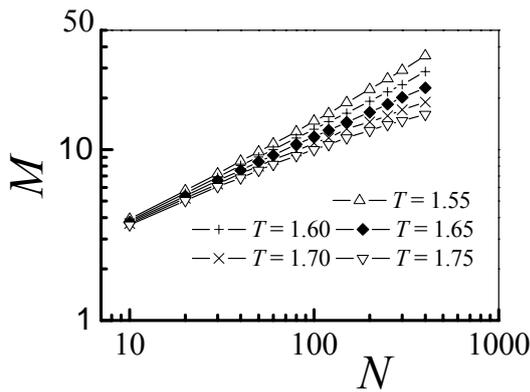


Figure 3 The dependence of the surface contact number  $M$  on the chain length  $N$ .

The two different situations are apparent in Fig. 3. It can be seen that the curve is concave upward when  $T \in (1.55, 1.60)$ , but downward convex curve when  $T \in (1.70, 1.75)$ . Therefore, the critical adsorption point  $T_c$  can be further determined in the interval  $T \in (1.60, 1.70)$ . The above phenomenon can be explained that the  $M - N$  curve is showing different when  $T$  is greater or less than  $T_c$ . The relationship between  $M$  and  $N$  can be expressed as

$$M = N^\phi (c_0 + c_1(T - T_c) + O((c_1(T - T_c))^2)). \quad (5)$$

Since the second item  $c_1(T - T_c)$  in the right of (5) changes the sign when  $T$  changes from  $T > T_c$  to  $T < T_c$ .

### C. Interpolation Method

In the interval  $[1.55, 1.75]$ , we want to get the surface contact number  $M$  with the temperature step  $\Delta T = 0.001$ . However, it takes a very long calculation time to simulate such a multi-temperature sample. In order to reduce the

simulation time, values of  $M$  at different temperatures are using quadratic interpolation to approximate from the five temperatures  $T = 1.55, 1.60, 1.65, 1.70, \text{ and } 1.75$ .

We use the equidistant interpolation for different chain length  $N = N_j$  included in the range  $[10, 400]$ . The values  $M = f_M(T_i, N_j)$  are known at the  $n$  equidistant temperatures,  $T_i = T_0 + ih$  ( $i = 0, 1, \dots, n - 1$ ) where  $T_0 = 1.55, h = 0.05, n = 5$ . The surface contact number  $M$  is calculated by using the parabolic interpolation formula for  $T \in (1.55, 1.75)$  with  $\Delta T = 0.001$ . In order to distinguish between the previous variables  $T_i$ , we use another symbol  $T'$  to present the temperature, which means that the calculated temperature values  $T'_k$  to be interpolated,  $T'_k = T_0 + k \Delta T$  ( $k = 0, 1, \dots, (T_{n-1} - T_0) / \Delta T$ ), where  $T_0 = 1.55, T_{n-1} = 1.75, \Delta T = 0.001$ . In order to calculate an approximation of  $M$  at temperature  $T = T'_k$ , the three temperatures are selected near the interpolation point  $T = T'_k$ . In the case of  $T_i < T'_k < T_{i+1}$ , if  $|T_i - T'_k| > |T'_k - T_{i+1}|$ , three temperatures  $T_i, T_{i+1}$ , and  $T_{i+2}$  are selected and if  $|T_i - T'_k| < |T'_k - T_{i+1}|$ , three temperatures  $T_{i-1}, T_i$ , and  $T_{i+1}$  are selected. Then the approximation of the surface contact number  $M$  is calculated by parabolic interpolation formula, which can be described as

$$\begin{aligned} & \text{if } (T_i < T'_k < T_{i+1}) \\ & \quad \{ \text{if } (|T_i - T'_k| > |T'_k - T_{i+1}|) \\ & \quad \quad t = k; \\ & \quad \text{else} \\ & \quad \quad t = k - 1; \\ & \quad M = \sum_{i=t}^{t+2} M(T_i) \prod_{j=t, j \neq i}^{t+2} [(T'_k - T_j) / (T_i - T_j)] \\ & \quad \}. \end{aligned}$$

### D. Fitting Curve $M = a_0 N^\phi$

When  $T_c = T'_k$ , there is a relationship  $M = a_0 N^\phi$ . For every temperature  $T'_k$ , there are a set of corresponding data  $(N_j, f_M(T'_k, N_j))$ . For these data  $(N, M)$ , we fit the curve  $M = a_0 N^\phi$ . If we set  $\bar{M} = \ln M, \bar{a}_0 = \ln a_0$  and  $\bar{N} = \ln N$ , the curve is changed to linear fitting  $\bar{M} = \bar{a}_0 + \phi \bar{N}$ . We use the least squares method, which can be expressed as

$$g(T'_k, \bar{a}_0(T'_k), \phi(T'_k)) = \sum_j (\ln f_M(T'_k, N_j) - \bar{a}_0(T'_k) - \phi(T'_k) \ln N_j). \quad (6)$$

For  $\frac{\partial g}{\partial (\bar{a}_0(T'_k))} = \frac{\partial g}{\partial (\phi(T'_k))} = 0$ , which can be expressed as

$$\frac{\partial g}{\partial (\bar{a}_0(T'_k))} = -2 \sum_{j=1}^n (\ln f_M(T'_k, N_j) - \bar{a}_0(T'_k) - \phi(T'_k) \ln N_j), \quad (7)$$

$$\frac{\partial g}{\partial (\phi(T'_k))} = -2 \sum_{j=1}^n (\ln f_M(T'_k, N_j) - \bar{a}_0(T'_k) - \phi(T'_k) \ln N_j) \ln N_j. \quad (8)$$

Solution of the equation can be expressed as

$$\bar{a}_0(T'_k) = \frac{\sum_{j=1}^n \ln^2 N_j \sum_{j=1}^n \ln f_M(T'_k, N_j) - \sum_{j=1}^n \ln N_j \sum_{j=1}^n \ln N_j \ln f_M(T'_k, N_j)}{n \sum_{j=1}^n \ln^2 N_j - (\sum_{j=1}^n \ln N_j)^2}, \quad (9)$$

$$\phi(T'_k) = \frac{n \sum_{j=1}^n \ln N_j \ln f_M(T'_k, N_j) - \sum_{j=1}^n \ln N_j \sum_{j=1}^n \ln f_M(T'_k, N_j)}{n \sum_{j=1}^n \ln^2 N_j - (\sum_{j=1}^n \ln N_j)^2}. \quad (10)$$

$a_0(T'_k)$  can be obtained from (9), which can be expressed as

$$a_0(T'_k) = \exp(\bar{a}_0(T'_k)). \quad (11)$$

Fitting formula can be expressed as

$$g_M(T'_k, N_j) = a_0(T'_k) N_j^{\phi(T'_k)}. \quad (12)$$

**E. Variance (between Interpolation and Fitting value), to Determine Crossover-exponent**

We calculate the variance between the interpolation value and the fitting value, which can be expressed as

$$\sigma^2(T'_k) = \sum_{j=1}^n \sigma_j^2 = \sum_{j=1}^n (f_M(T'_k, N_j) - g_M(T'_k, N_j))^2. \quad (13)$$

The temperature where the variance is a minimum is the critical adsorption point, as shown in Fig. 4.

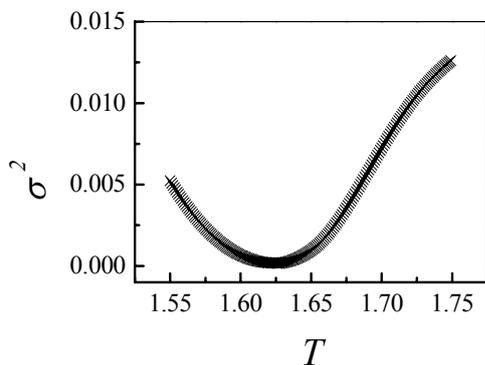


Figure 4 The variance between the interpolation value and the fitting value.

We get  $T_c = 1.625$ ,  $\phi = 0.52$  calculated respectively by the formulas, which are expressed as

$$T_c = \{T'_k \mid \text{where } \min_{k=0}^{(T_{n+1}-T_0)/\Delta T} (\sigma^2(T'_k))\}, \quad (14)$$

and

$$\phi = \{\phi(T'_k) \mid T'_k = T_c\}. \quad (15)$$

**F. Another Critical Exponent  $\delta$**

$MN^{-\phi}$  can be obtained from (5) divided by  $N^\phi$  on both left and right sides, which can be expressed as

$$MN^{-\phi} = c_0 + c_1(T - T_c) + c_2(T - T_c)^2. \quad (16)$$

The dependence of  $MN^{-\phi}$  on  $(T - T_c)$  is listed for chain length from  $N = 10$  to  $N = 400$  near the critical adsorption point  $T_c$  in Fig. 5. Near at  $T_c$ , the curves can be expressed by a second order polynomial which is defined as

$$MN_j^{-\phi} = a_0 + c_1(N_j)(T - T_c) + c_2(N_j)(T - T_c)^2. \quad (17)$$

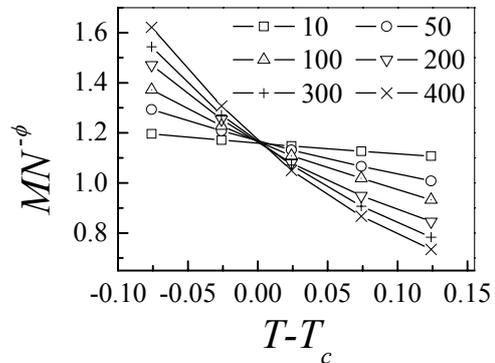


Figure 5 The relationship between  $MN^{-\phi}$  and  $T - T_c$ .

We can calculate the coefficient  $c_1(N_j)$  using (17) to fit the curves between the relationship  $(T - T_c)$  and  $MN_j^{-\phi}$ . The dependence of  $c_1(N)$  on  $N$  is shown in Fig. 6. We can get  $c_1(N) = a_1 N^{1/\delta}$ . Then we calculated another critical exponent  $\delta = 1.63$ . There is only one critical exponent in EKB scaling method [6], which is equivalent to our scaling method  $\delta = 1/\phi$ . However, we found that  $1/\delta$  is not close to  $\phi$  in the scaling method. Whether it is efficient that we get two critical exponents  $\phi$ ,  $\delta$  and the critical adsorption point  $T_c$ .

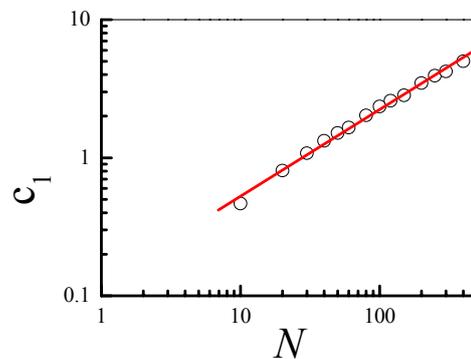


Figure 6 The relationship between the coefficient  $c_1$  and the chain length  $N$ .

The dependence of  $MN^{-\phi}$  on  $(T - T_c)N^{1/\delta}$  is calculated for chain length  $N \in [10, 400]$  near  $T_c$ , as shown in Fig. 7. These curves are satisfied by the relationship which can be expressed as

$$MN^{-\phi} = (a_0 + a_1(T - T_c)N^{1/\delta} + O(((T - T_c)N^{1/\delta})^2)). \quad (18)$$

We obtain

$$M = N^\phi (a_0 + a_1(T - T_c)N^{1/\delta} + O(((T - T_c)N^{1/\delta})^2)) \quad (19)$$

by multiplying  $N^\phi$  on both sides of (18) near the critical adsorption point  $T_c$ . We found that two critical exponents present well the properties near at  $T_c$ .

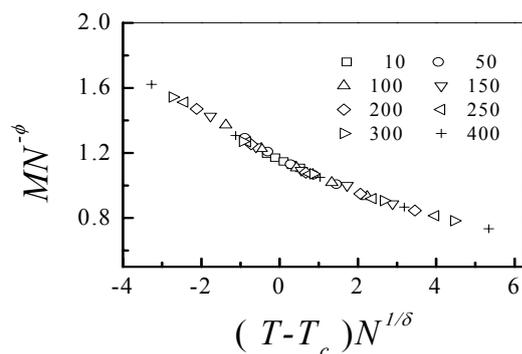


Figure 7 The dependence of  $MN^{-\phi}$  on  $(T-T_c)N^{1/\delta}$ .

#### IV. CONCLUSIONS

The polymer chain is generated by self-avoiding walk in the simulation. The chain movement is simulated by bond-fluctuation model. The attraction interaction between the polymer chain and the surface is related to the temperature  $T$ . The critical adsorption point  $T_c$  is calculated by scaling between the surface contact number  $M$  and the chain length  $N$ . Using the interpolation method replace simulating large samples, which is to ensure highly accurate and to reduce the computation time. Our scale algorithm represents well properties of the polymer chain by two critical exponents  $\phi$  and  $\delta$  near at the critical adsorption point  $T_c$ . The scaling algorithm provides a new method to determine the critical adsorption point and the critical exponents.

#### ACKNOWLEDGMENT

This work was supported in part by the National Science Foundation of China under Grant No. 11304231. We thank Shandong University High Performance Computing Center and Wenzhou University High Performance Computing Center.

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